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Supplementary material

Guidelines to multivariate assessment of chromatographic lipophilicity scales – reversed phase thin-layer chromatography

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Table S1 List of studied compounds accompanied with Abraham's solvatochromic parameters (*A* – hydrogen bond proton donating ability, *B* – hydrogen bond proton accepting ability, *S* – dipolarity, *E* – polarizability, *V* – McGowan's molar molecular volume); Acidity constants p*K*a; Ionization degree α at pH = 6; Molar mass; Water solubility (log *S*)

No	Compound	logK_{OW} (exp)	Determination method[b]	Ref.	*M* (g/mol)	Solvatochromic parameters					log*S*[c]	Ref.	p*K*a	Ref.	α (%)[e] pH = 6
						A	*B*	*S*	*E*	*V*					
1	Phenol	1.46[a]	SF	A1	94.12	0.60	0.30	0.89	0.81	0.775	-0.06	B1	9.99	C1	0.01
2	4-Nitrophenol	1.91[a]	SF	A1	139.12	0.82	0.26	1.72	1.07	0.949	-1.08	B2	7.18	C1	**6.20**
3	Benzyl Alcohol	1.10[a]	SF	A1	109.14	0.39	0.56	0.87	0.80	0.916	-0.41	B3	-	-	-
4	1-Naphthylamine	2.25[a]	SF	A1	143.20	0.20	0.57	1.26	1.67	1.185	-1.93	B4	3.92[d]	C2	99.18
5	1-Naphthol	2.85[a]	SF	A1	144.18	0.60	0.37	1.05	1.52	1.144	-2.22	B5	9.34	C3	0.05
6	2,4-Dichlorophenol	3.06[a]	SF	A1	163.00	0.53	0.19	0.84	0.96	1.020	-1.56	B3	7.65	C1	2.19
7	Anthracene	4.45[a]	SF	A1	178.24	0.00	0.28	1.34	2.29	1.454	-6.61	B6	-	-	-
8	Acetophenone	1.58[a]	SF	A1	120.16	0.00	0.48	1.01	0.82	1.014	-1.29	B1	-	-	-
9	2,4,6-Trichlorophenol	3.69[a]	-	A1	197.45	0.42	0.15	0.94	1.07	1.142	-2.39	B7	6.42	C1	**27.55**
10	Ethyl-*p*-hydroxybenzoate	2.47[a]	-	A1	166.19	0.69	0.45	1.35	0.86	1.272	-2.27	B8	8.5	C4	0.32
11	*p*-Anisidine	0.95[a]	SF	A1	123.17	0.16	0.66	1.26	1.05	1.016	-0.77	B9	5.36[d]	C5	81.36
12	1,2,3-benzotriazole	1.44[a]	-	A1	119.14	0.62	0.48	1.70	1.47	0.864	-0.78	B10	8.37	C3	0.42
13	Diphenylamine	3.50[a]	-	A1	169.24	0.08	0.51	1.08	1.59	1.424	-3.50	B8	0.78[d]	C6	100.00
14	2,2'-Bipyridyl	1.50	SF	A2	156.20	0.00	0.81	1.33	1.38	1.242	-1.42	B3	4.33[d]	C7	97.91
15	4-Bromoaniline	2.26[a]	SF	A1	172.03	0.31	0.30	1.19	1.19	0.991	**-1.47**	B11	3.86[d]	C8	99.28
16	Benzophenone	3.18[a]	-	A1	182.23	0.00	0.50	1.50	1.45	1.481	-3.12	B3	-	-	-
17	4-Aminobenzoic acid	0.83[a]	SF	A1	137.15	0.94	0.69	1.61	1.08	1.032	-1.35	B8	2.38	C9	**99.98**
18	Pyrene	4.88[a]	SF	A1	202.26	0.00	0.25	1.52	2.60	1.585	-6.18	B12	-	-	-
19	Benzo(a)pyrene	6.13	SS	A3	252.32	0.00	0.31	1.84	3.32	1.954	-8.19	B6	-	-	-
20	Fluorene	4.18[a]	SF	A1	166.23	0.00	0.25	1.06	1.59	1.357	-4.99	B13	-	-	-
21	Acenaphthene	3.92[a]	SF	A1	154.22	0.00	0.26	1.14	1.75	1.259	-4.60	B12	-	-	-
22	Naphthalene	3.30[a]	-	A1	128.18	0.00	0.20	0.92	1.34	1.085	-3.62	B14	-	-	-
23	Phenanthrene	4.46[a]	SF	A1	178.24	0.00	0.29	1.29	2.06	1.454	-5.19	B15	-	-	-
24	Dibenz(a,h)anthracene	6.50[a]	SF	A4	278.36	0.00	0.35	1.99	3.43	2.192	-8.05	B5	-	-	-
25	Benz(a)anthracene	5.76	HPLC	A5	228.30	0.00	0.29	1.66	2.71	1.823	-7.39	B16	-	-	-
26	Simazine	2.18[a]	-	A1	201.69	0.33	0.95	1.20	1.55	1.479	-4.51	B17	1.62[d]	C10	100.00
27	Propazine	2.93[a]	-	A1	229.75	0.30	0.97	1.14	1.47	1.761	-4.43	B8	1.85[d]	C10	99.99
28	Ametryn	2.98[a]	-	A1	227.38	0.26	1.07	1.27	1.50	1.802	-3.04	B8	4.10[d]	C11	98.76
29	Prometryn	3.51[a]	-	A1	241.41	0.26	1.10	1.26	1.51	1.940	-3.86	B18	4.05[d]	C11	98.89
30	3-Nitrophenol	2.00[a]	SF	A1	139.12	0.79	0.23	1.57	1.05	0.949	-1.01	B8	8.36	C1	0.43
31	2-Naphthol	2.70[a]	SF	A1	144.18	0.61	0.40	1.08	1.52	1.144	-2.28	B3	9.67	C12	0.02

No	Compound	logK_{OW} (exp)	Determination method[b]	Ref.	M (g/mol)	Solvatochromic parameters					log$S$[c]	Ref.	pKa	Ref.	α (%)[e] pH = 6
						A	B	S	E	V					
32	4-Hydroxybenzaldehyde	1.35[a]	-	A1	122.13	0.85	0.37	1.54	1.01	0.932	-1.16	B19	7.61	C3	2.40
33	2-Aminophenol	0.62[a]	-	A1	109.14	0.60	0.66	1.10	1.11	0.875	-0.74	B3	9.44 (-OH)	C1	0.04
34	4-*t*-Butylphenol	3.31[a]	-	A1	150.24	0.56	0.41	0.89	0.81	1.339	-2.41	B3	10.31	C1	0.00
35	2,6-Dimethylphenol	2.36[a]	SF	A1	122.18	0.39	0.39	0.79	0.86	1.057	-1.31	B3	10.59	C1	0.00
36	4-Methoxyphenol	1.58[a]	SF	A1	124.15	0.57	0.48	1.17	0.90	0.975	**-0.49**	B11	10.27	C1	0.01
37	Methyl-*p*-hydroxybenzoate	1.96[a]	-	A1	152.16	0.69	0.45	1.37	0.90	1.131	-1.78	B8	8.47	C4	0.34
38	2-Nitrobenzaldehyde	1.74[a]	-	A1	151.13	0.00	0.38	1.59	1.12	1.047	-1.81	B20	-	-	-
39	3-Nitrobenzaldehyde	1.46[a]	-	A1	151.13	0.00	0.48	1.49	1.10	1.047	-1.97	B20	-	-	-
40	Phthalimide	1.15[a]	-	A1	147.14	0.39	0.44	1.97	1.18	1.021	-2.61	B3	8.3	C13	0.50
41	Oxazepam	2.24[a]	SF	A1	286.73	0.45	1.60	1.10	2.35	1.992	**-3.65**	B11	10.9 (-OH)	C14	0.00
42	Lorazepam	2.39[a]	SF	A1	321.18	0.45	1.63	1.28	2.51	2.114	-3.60	B21	11.5 (-OH)	C15	0.00
43	Clonazepam	2.41[a]	SF	A1	315.73	0.33	1.50	1.75	2.46	2.107	-3.50	B21	10.5 (-OH)	C16	0.00
44	Bromazepam	2.05	SF	A6	316.17	0.33	1.62	1.38	2.31	1.940	**-3.25**	B11	11.0 (-OH)	C17	0.00
45	Diazepam	2.82[a]	-	A1	284.76	0.00	1.25	1.57	2.08	2.074	-3.76	B3	3.40[d]	C18	99.75
46	Nitrazepam	2.25[a]	SF	A1	281.29	0.47	1.10	2.17	2.21	1.985	**-5.14**	B11	10.8	C15	0.00
47	Chlordiazepoxide	2.44[a]	-	A1	299.78	0.13	0.94	1.65	1.95	2.174	-2.18	B3	4.80[d]	C18	94.06
48	Clobazam	2.12	SF	A7	300.76	0.00	1.47	2.49	2.29	2.133	**-2.19**	B11	6.65[d]	C19	18.29
49	Medazepam	4.41[a]	SF	A1	270.78	0.00	0.67	1.40	1.92	2.058	**-5.85**	B11	6.20[d]	C20	38.69
50	Chrysene	5.81	SS	A3	228.30	0.00	0.29	1.66	2.71	1.823	-8.06	B12	-	-	-

[a]log K_{OW} values recommended by C. Hansch and A. Leo

[b]Octanol-water partition coefficient determination method: SF - shake flask, SS - slow stirring, HPLC - High Performance Liquid Chromatography

[c]Computationally estimated water solubility by fragment-based methods are marked in bold. The rest of the data are experimentally determined values under different conditions, taken from the EPI Suite v4.03 database (WATERNT® v. 1.01) – U.S. EPA

[d]Ionization degrees (α) for compounds that are present in charged forms under the studied chromatographic conditions are marked in bold

Table S2a List of chromatographic lipophilicity indices (R_M^0, b, C_0, $PC1/R_M$, mR_M); Chromatographic systems - stationary phase: **octadecyl-modified silica**; mobile phase: a) methanol-water and b) acetonitrile-water

No	Compound	MeOH-water					MeCN-water				
		R_M^0	b[a]	C^0	mR_M	$PC1/R_M$ (94.11%)[b]	R_M^0	b[a]	C_0	mR_M	$PC1/R_M$ (97.94%)[b]
1	Phenol	1.474	0.0234	63.10	0.072	-2.464	1.832	0.0338	54.27	-0.194	-2.076
2	4-Nitrophenol	1.631	0.0240	67.99	0.192	-1.990	1.858	0.0337	55.18	-0.162	-1.942
3	Benzyl Alcohol	1.546	0.0240	64.48	0.107	-2.323	1.426	0.0275	51.78	-0.226	-2.200
4	1-Naphthylamine	2.538	0.0330	76.89	0.557	-0.565	2.154	0.0315	68.39	0.264	-0.123
5	1-Naphthol	2.889	0.0374	77.35	0.648	-0.220	2.267	0.0343	66.02	0.207	-0.374
6	2,4-Dichlorofenol	2.843	0.0354	80.28	0.718	0.057	2.200	0.0328	67.00	0.230	-0.272
7	Anthracene	3.711	0.0376	98.68	1.351	2.604	2.982	0.0333	89.54	0.984	2.934
8	Acetophenone	2.137	0.0289	73.86	0.401	-1.177	1.778	0.0275	64.60	0.127	-0.698
9	2,4,6-Trichlorophenol	2.796	0.0330	84.85	0.819	0.486	2.130	0.0288	73.85	0.399	0.459
10	Ethyl-*p*-hydroxybenzoate	2.441	0.0332	73.47	0.448	-1.008	1.866	0.0318	58.76	-0.039	-1.414
11	*p*-Anisidine	1.494	0.0231	64.77	0.110	-2.313	1.431	0.0245	58.28	-0.042	-1.408
12	1,2,3-benzotriazole	1.436	0.0238	60.36	0.008	-2.725	1.561	0.0329	47.41	-0.415	-3.014
13	Diphenylamine	2.883	0.0333	86.48	0.883	0.726	3.050	0.0397	76.83	0.668	1.575
14	2,2'-Bipyridyl	2.359	0.0307	76.92	0.519	-0.705	1.448	0.0192	75.42	0.296	0.045
15	4-Bromoaniline	2.374	0.0314	75.73	0.493	-0.817	2.029	0.0303	66.93	0.210	-0.349
16	Benzophenone	3.231	0.0391	82.54	0.882	0.710	2.802	0.0365	76.71	0.610	1.337
17	4-Aminobenzoic acid	0.113	0.0107	10.55	-0.531	-4.833	0.740	0.0234	31.66	-0.663	-4.045
18	Pyrene	4.396	0.0451	97.38	1.493	3.179	3.000	0.0319	94.05	1.086	3.374
19	Benzo(a)pyrene	4.394	0.0392	112.21	1.804	4.455	3.179	0.0305	104.31	1.350	4.502
20	Fluorene	3.102	0.0315	98.60	1.192	1.977	2.999	0.0355	84.40	0.867	2.432
21	Acenaphthene	3.990	0.0453	88.00	1.270	2.212	3.249	0.0400	81.22	0.849	2.343
22	Naphthalene	4.125	0.0487	84.74	1.204	1.943	2.612	0.0327	79.89	0.650	1.518
23	Phenanthrene	3.723	0.0379	98.24	1.449	2.960	3.024	0.0335	90.35	1.016	3.069
24	Dibenz(a,h)anthracene	3.678	0.0340	108.19	1.582	3.534	3.071	0.0286	107.40	1.355	4.526
25	Benz(a)anthracene	3.628	0.0319	113.73	1.651	3.824	3.592	0.0383	93.73	1.293	4.236
26	Simazine	2.897	0.0381	76.00	0.610	-0.373	1.760	0.0265	66.41	0.170	-0.511
27	Propazine	3.852	0.0480	80.32	0.974	1.048	2.385	0.0322	74.15	0.455	0.688
28	Ametryn	3.371	0.0400	84.36	0.973	1.067	2.032	0.0272	74.69	0.400	0.465
29	Prometryn	3.338	0.0376	88.70	1.080	1.494	2.472	0.0317	78.02	0.571	1.181

No	Compound	MeOH-water					MeCN-water				
		R_M^0	b^a	C^0	mR_M	$PC1/R_M$ (94.11%)[b]	R_M^0	b^a	C_0	mR_M	$PC1/R_M$ (97.94%)[b]
30	3-Nitrophenol	1.934	0.0279	69.40	0.262	-1.720	1.821	0.0330	55.23	-0.157	-1.920
31	2-Naphthol	2.906	0.0384	75.65	0.601	-0.406	2.079	0.0335	62.11	0.071	-0.952
32	4-Hydroxybenzaldehyde	1.400	0.0242	57.74	-0.055	-2.966	1.544	0.0331	46.69	-0.440	-3.123
33	2-Aminophenol	1.080	0.0208	51.91	-0.168	-3.414	1.376	0.0293	46.98	-0.381	-2.864
34	4-*t*-Butylphenol	3.454	0.0430	80.36	0.875	0.664	2.277	0.0333	68.48	0.282	-0.051
35	2,6-Dimethylphenol	2.312	0.0302	76.52	0.499	-0.787	2.012	0.0311	64.69	0.146	-0.625
36	4-Methoxyphenol	1.524	0.0253	60.29	0.007	-2.722	1.598	0.0317	50.34	-0.307	-2.552
37	Methyl-*p*-hydroxybenzoate	2.123	0.0313	67.72	0.242	-1.810	1.628	0.0308	52.91	-0.218	-2.172
38	2-Nitrobenzaldehyde	2.273	0.0339	67.01	0.238	-1.831	1.851	0.0299	61.96	0.059	-0.993
39	3-Nitrobenzaldehyde	2.009	0.0290	69.24	0.268	-1.700	1.826	0.0297	61.40	0.042	-1.065
40	Phthalimide	1.667	0.0265	62.99	0.079	-2.443	1.379	0.0278	49.64	-0.288	-2.460
41	Oxazepam	3.219	0.0418	76.97	0.710	0.007	1.772	0.0299	59.25	-0.022	-1.338
42	Lorazepam	3.350	0.0442	75.86	0.700	-0.048	1.835	0.0307	59.83	-0.005	-1.267
43	Clonazepam	3.208	0.0428	74.90	0.638	-0.276	2.027	0.0329	61.55	0.051	-1.033
44	Bromazepam	2.949	0.0394	74.79	0.583	-0.481	1.382	0.0222	62.18	0.049	-1.017
45	Diazepam	3.202	0.0371	86.29	0.976	1.091	2.332	0.0298	78.23	0.543	1.069
46	Nitrazepam	3.019	0.0399	75.64	0.624	-0.327	1.974	0.0322	61.23	0.040	-1.081
47	Chlordiazepoxide	3.242	0.0428	75.72	0.673	-0.140	1.933	0.0318	60.78	0.025	-1.142
48	Clobazam	3.558	0.0465	76.58	0.770	0.234	2.173	0.0322	67.47	0.241	-0.225
49	Medazepam	4.370	0.0431	101.29	1.660	3.824	3.219	0.0316	101.94	1.324	4.387
50	Chrysene	4.557	0.0415	109.89	1.814	4.489	3.425	0.0358	95.57	1.275	4.167

[a]The slope *b* was multiplied by -1 in order to be positively correlated with the rest of lipophilicity measures

[b]Percent of data variability captured by the first principal component

Table S2b Chromatographic descriptors used as lipophilicity indices (R_M^0, b, C_0, $PC1/R_M$, mR_M). Chromatographic systems - stationary phase: **cyano-modified silica**; mobile phase: a) methanol-water and b) acetonitrile-water

No	Compound	MeOH-water					MeCN-water				
		R_M^0	b[a]	C^0	mR_M	$PC1/R_M$ (97.87%)[b]	R_M^0	b[a]	C_0	mR_M	$PC1/R_M$ (96.92%)[b]
1	Phenol	0.584	0.0159	36.70	-0.291	-1.881	0.910	0.0246	36.97	-0.321	-2.389
2	4-Nitrophenol	1.122	0.0210	53.33	-0.035	-0.663	1.108	0.0262	42.21	-0.204	-1.529
3	Benzyl Alcohol	0.369	0.0142	26.04	-0.410	-2.461	0.694	0.0213	32.59	-0.371	-2.740
4	1-Naphthylamine	1.387	0.0223	62.26	0.162	0.316	1.335	0.0257	51.89	0.049	0.391
5	1-Naphthol	1.604	0.0264	60.65	0.149	0.198	1.378	0.0279	49.41	-0.017	-0.129
6	2,4-Dichlorofenol	1.564	0.0271	57.78	0.075	-0.190	1.626	0.0328	49.57	-0.014	-0.155
7	Anthracene	2.749	0.0375	73.24	0.685	2.737	2.020	0.0331	60.98	0.364	2.702
8	Acetophenone	0.828	0.0182	45.44	-0.174	-1.330	1.260	0.0286	44.11	-0.168	-1.276
9	2,4,6-Trichlorophenol	1.758	0.0289	60.86	0.169	0.258	1.996	0.0380	52.54	0.097	0.630
10	Ethyl-*p*-hydroxybenzoate	1.029	0.0219	46.95	-0.176	-1.391	1.234	0.0290	42.60	-0.214	-1.635
11	*p*-Anisidine	0.918	0.0129	71.12	0.208	0.671	1.422	0.0271	52.51	0.068	0.530
12	1,2,3-benzotriazole	0.336	0.0128	26.23	-0.369	-2.236	0.588	0.0194	30.26	-0.383	-2.810
13	Diphenylamine	2.261	0.0334	67.65	0.423	1.480	2.474	0.0431	57.43	0.320	2.261
14	2,2'-Bipyridyl	0.639	0.0155	41.37	-0.211	-1.473	0.904	0.0200	45.30	-0.094	-0.630
15	4-Bromoaniline	1.135	0.0202	56.17	0.024	-0.352	1.256	0.0257	48.81	-0.031	-0.210
16	Benzophenone	1.753	0.0292	59.96	0.145	0.137	1.144	0.0258	44.35	-0.146	-1.081
17	4-Aminobenzoic acid	0.172	0.0116	14.79	-0.468	-2.719	1.668	0.0363	45.89	-0.149	-1.218
18	Pyrene	3.153	0.0430	73.33	0.788	3.199	2.741	0.0445	61.57	0.515	3.729
19	Benzo(a)pyrene	3.261	0.0404	80.63	1.037	4.470	2.973	0.0466	63.81	0.643	4.676
20	Fluorene	2.631	0.0384	68.47	0.518	1.895	2.227	0.0383	58.18	0.313	2.253
21	Acenaphthene	2.477	0.0365	67.82	0.468	1.671	2.100	0.0367	57.25	0.266	1.920
22	Naphthalene	2.389	0.0355	67.34	0.438	1.534	1.964	0.0345	56.94	0.239	1.740
23	Phenanthrene	2.870	0.0409	70.23	0.622	2.385	2.429	0.0414	58.63	0.357	2.561
24	Dibenz(a,h)anthracene	3.230	0.0404	80.01	1.010	4.332	2.886	0.0451	63.94	0.629	4.584
25	Benz(a)anthracene	3.138	0.0403	77.91	0.923	3.892	2.738	0.0437	62.72	0.555	4.037
26	Simazine	1.000	0.0206	48.42	-0.136	-1.169	0.917	0.0216	42.45	-0.163	-1.160
27	Propazine	1.466	0.0269	54.61	-0.010	-0.621	2.139	0.0403	53.11	0.125	0.813
28	Ametryn	1.438	0.0263	54.60	-0.010	-0.618	0.790	0.0150	52.63	0.040	0.430
29	Prometryn	1.674	0.0293	57.14	0.063	-0.287	0.854	0.0155	55.14	0.080	0.728
30	3-Nitrophenol	1.114	0.0225	49.53	-0.123	-1.131	0.665	0.0194	34.25	-0.306	-2.232

No	Compound	MeOH-water					MeCN-water				
		R_M^0	b^a	C^0	mR_M	$PC1/R_M$ (97.87%)[b]	R_M^0	b^a	C_0	mR_M	$PC1/R_M$ (96.92%)[b]
31	2-Naphthol	1.428	0.0259	55.14	0.004	-0.537	0.748	0.0187	39.99	-0.187	-1.329
32	4-Hydroxybenzaldehyde	0.544	0.0166	32.80	-0.368	-2.282	0.465	0.0185	25.09	-0.461	-3.399
33	2-Aminophenol	0.533	0.0122	43.87	-0.135	-1.049	0.695	0.0174	39.84	-0.177	-1.230
34	4-*t*-Butylphenol	1.557	0.0299	52.03	-0.089	-1.061	1.790	0.0340	52.59	0.088	0.624
35	2,6-Dimethylphenol	1.084	0.0224	48.48	-0.146	-1.244	1.588	0.0317	50.17	0.005	0.009
36	4-Methoxyphenol	0.466	0.0142	32.71	-0.317	-1.996	0.857	0.0239	35.94	-0.335	-2.490
37	Methyl-*p*-hydroxybenzoate	0.755	0.0190	39.71	-0.291	-1.925	0.845	0.0237	35.59	-0.342	-2.541
38	2-Nitrobenzaldehyde	0.741	0.0169	43.79	-0.190	-1.387	0.906	0.0208	43.56	-0.134	-0.932
39	3-Nitrobenzaldehyde	0.894	0.0185	48.44	-0.121	-1.064	0.894	0.0209	42.84	-0.149	-1.047
40	Phthalimide	0.673	0.0183	36.74	-0.334	-2.142	0.633	0.0203	31.17	-0.382	-2.801
41	Oxazepam	1.192	0.0245	48.75	-0.153	-1.309	1.092	0.0274	39.91	-0.276	-2.067
42	Lorazepam	1.311	0.0261	50.13	-0.127	-1.203	1.189	0.0284	41.87	-0.231	-1.734
43	Clonazepam	1.572	0.0273	57.47	0.067	-0.240	1.318	0.0287	45.93	-0.117	-0.871
44	Bromazepam	0.867	0.0198	43.76	-0.223	-1.594	0.887	0.0229	38.70	-0.259	-1.896
45	Diazepam	1.660	0.0285	58.20	0.091	-0.135	1.424	0.0282	50.56	0.016	0.140
46	Nitrazepam	1.476	0.0253	58.30	0.084	-0.129	1.222	0.0273	44.71	-0.144	-1.062
47	Chlordiazepoxide	1.475	0.0254	57.98	0.076	-0.170	1.249	0.0275	45.43	-0.126	-0.932
48	Clobazam	1.529	0.0264	57.90	0.077	-0.180	1.345	0.0281	47.90	-0.059	-0.423
49	Medazepam	3.321	0.0418	79.48	1.023	4.390	2.995	0.0485	61.73	0.569	4.114
50	Chrysene	4.549	0.0623	73.07	1.125	4.606	3.329	0.0525	63.36	0.702	5.076

[a] The slope *b* was multiplied by -1 in order to be positively correlated with the rest of lipophilicity measures

[b] percent of data variability captured by the first principal component

Table S3 Computationally estimated logK_{OW} (log$P$) values

No	Compound	ALOGPs	AClogP	ACDlogP	AB/LogP	miLogP	ALOGP	ClogP	MLOGP	KOWIN	XLOGP2	XLOGP3	LSER
1	Phenol	1.39	1.68	1.48	1.41	1.46	1.56	1.48	1.51	1.51	1.62	1.46	1.54
2	4-Nitrophenol	1.93	1.69	1.57	1.73	1.42	1.46	1.85	1.35	1.91	1.51	1.91	1.63
3	Benzyl Alcohol	1.07	1.36	1.03	1.26	1.27	1.23	1.10	1.59	1.08	1.21	1.10	1.19
4	1-Naphthylamine	2.27	2.44	2.17	2.26	2.58	1.99	2.09	2.64	2.25	2.47	2.25	2.25
5	1-Naphthol	2.79	2.86	2.71	2.95	2.88	2.47	2.65	2.64	2.85	2.88	2.84	2.94
6	2,4-Dichlorofenol	3.14	2.91	2.99	3.21	3.00	2.89	2.97	2.73	2.80	2.86	3.06	2.99
7	Anthracene	4.56	4.34	4.68	4.40	4.30	3.65	4.49	4.33	4.35	4.55	4.45	4.54
8	Acetophenone	1.65	1.90	1.66	1.62	1.84	1.57	1.58	2.10	1.67	1.86	1.58	1.69
9	2,4,6-Trichlorophenol	3.78	3.52	3.58	3.79	3.61	3.56	3.39	3.31	3.45	3.48	3.69	3.55
10	Ethyl-*p*-hydroxybenzoate	2.76	2.09	2.40	2.37	2.00	1.77	2.51	1.78	2.47	1.98	2.47	2.47
11	*p*-Anisidine	1.01	1.15	0.74	1.02	1.07	1.07	1.00	1.25	1.16	1.12	0.95	0.95
12	1,2,3-benzotriazole	1.19	0.95	1.34	1.66	1.29	1.43	1.41	1.05	1.17	1.14	1.44	0.78
13	Diphenylamine	3.34	3.86	2.97	3.80	3.93	3.38	3.62	3.39	3.29	3.23	3.50	3.51
14	2,2'-Bipyridyl	1.85	1.63	1.28	1.82	1.44	1.90	1.56	1.55	1.38	1.64	1.73	1.40
15	4-Bromoaniline	2.10	1.96	2.05	2.06	1.82	1.83	2.06	2.30	2.26	2.00	2.26	2.26
16	Benzophenone	3.03	3.25	3.18	2.98	3.39	3.23	3.18	3.59	3.15	3.58	3.43	3.24
17	4-Aminobenzoic acid	0.78	0.78	0.83	0.83	0.92	0.69	0.98	0.03	0.96	0.82	0.83	0.57
18	Pyrene	5.19	5.03	5.17	4.69	4.88	3.94	4.95	4.76	4.88	5.15	4.88	5.13
19	Benzo(a)pyrene	6.39	6.22	6.40	6.30	6.01	4.85	6.12	5.55	6.11	6.41	5.97	6.39
20	Fluorene	4.26	4.12	4.16	3.98	3.83	3.49	4.08	4.15	4.02	3.91	4.18	4.17
21	Acenaphthene	4.01	3.66	4.19	4.01	3.27	3.34	3.77	3.96	4.15	3.61	3.92	3.77
22	Naphthalene	3.33	3.16	3.45	3.37	3.15	2.74	3.32	3.39	3.17	3.29	3.30	3.32
23	Phenanthrene	4.55	4.34	4.68	4.72	4.30	3.65	4.49	4.33	4.35	4.55	4.46	4.43
24	Dibenz(a,h)anthracene	6.93	6.71	7.14	7.14	6.62	5.46	6.84	5.92	6.70	7.09	6.50	7.07
25	Benz(a)anthracene	5.72	5.53	5.91	5.87	5.46	4.55	5.66	5.16	5.52	5.82	5.79	5.81
26	Simazine	2.48	2.07	2.28	2.20	2.25	2.16	2.39	2.27	2.40	1.20	2.18	2.06
27	Propazine	2.94	2.88	2.98	2.96	2.85	2.91	3.01	2.89	3.24	2.12	2.93	3.08
28	Ametryn	3.09	2.36	3.09	3.01	3.02	2.74	3.20	2.59	3.32	1.78	2.98	2.77
29	Prometryn	3.31	2.77	3.44	3.39	3.32	3.12	3.51	2.89	3.73	2.24	3.51	3.21
30	3-Nitrophenol	1.92	1.69	1.93	1.94	1.39	1.46	1.85	1.35	1.91	1.51	2.00	1.88
31	2-Naphthol	2.93	2.86	2.71	2.95	2.64	2.47	2.65	2.64	2.69	2.88	2.70	2.80
32	4-Hydroxybenzaldehyde	1.27	1.37	1.39	1.56	1.25	1.32	1.44	1.16	1.23	1.31	1.35	1.33
33	2-Aminophenol	0.35	0.96	0.44	0.59	1.15	0.82	0.62	1.40	0.60	1.23	0.62	0.63
34	4-*t*-Butylphenol	3.47	3.20	3.77	3.36	3.16	2.96	3.30	2.81	3.42	3.43	3.31	3.31
35	2,6-Dimethylphenol	2.32	2.31	2.40	2.40	2.52	2.54	2.37	2.19	2.61	2.07	2.36	2.43

No	Compound	ALOGPs	AClogP	ACDlogP	AB/LogP	miLogP	ALOGP	ClogP	MLOGP	KOWIN	XLOGP2	XLOGP3	LSER
36	4-Methoxyphenol	1.31	1.58	1.31	1.51	1.51	1.55	1.57	1.25	1.58	1.53	1.34	1.44
37	Methyl-*p*-hydroxybenzoate	2.17	1.66	1.86	1.97	1.63	1.42	1.98	1.47	2.00	1.55	1.96	1.93
38	2-Nitrobenzaldehyde	1.36	1.67	1.74	1.53	1.64	1.48	1.78	1.61	1.74	1.61	1.74	1.72
39	3-Nitrobenzaldehyde	1.48	1.67	1.75	1.53	1.66	1.48	1.50	1.61	1.53	1.61	1.47	1.47
40	Phthalimide	0.83	1.01	1.15	1.11	1.44	0.66	1.15	1.38	1.30	0.99	1.15	1.06
41	Oxazepam	2.01	2.64	2.31	2.04	1.84	2.84	2.31	3.12	2.32	2.84	2.24	2.32
42	Lorazepam	2.98	3.25	2.47	2.52	2.47	3.50	2.37	3.36	2.41	3.47	2.39	2.59
43	Clonazepam	2.76	3.00	2.47	2.57	2.77	3.07	2.38	2.84	2.53	2.67	2.41	2.48
44	Bromazepam	2.09	2.10	1.65	-0.50	2.41	2.54	1.70	2.18	1.93	1.79	1.69	1.74
45	Diazepam	2.63	2.86	2.91	0.06	2.74	3.38	2.96	3.36	2.82	2.92	2.99	3.19
46	Nitrazepam	1.95	2.38	2.18	-0.50	2.14	2.41	2.32	2.59	2.45	2.05	2.25	2.82
47	Chlordiazepoxide	2.01	3.29	2.16	-0.34	2.12	2.03	2.47	3.69	2.42	3.39	2.14	4.49
48	Clobazam	2.14	3.17	1.69	-0.51	2.55	2.74	2.44	2.95	1.82	2.28	2.12	1.80
49	Medazepam	4.08	3.47	4.43	1.05	3.42	4.14	4.12	3.86	4.41	4.40	4.41	5.22
50	Chrysene	5.71	5.53	5.91	1.97	5.46	4.55	5.66	5.16	5.52	5.82	5.73	5.81

Table S4a Sum of ranking differences (SRD) scores of chromatographic and *in silico* lipophilicity measures using different data pretreatment methods: standardization (St), range scaling (Rg) and ranking (Rk)

St		**Rg**		**Rk**	
ClogP	9.28	logK_{OW}(exp)	9.28	logK_{OW}(exp)	9.12
logK_{OW}(exp)	9.44	ClogP	9.28	ClogP	9.6
XLOGP3	9.76	XLOGP3	9.92	R_M^0(CN-MeOH)	9.92
miLogP	9.92	miLogP	10.08	XLOGP3	10.24
R_M^0(CN-MeOH)	9.92	R_M^0(CN-MeOH)	10.08	LSER	10.4
LSER	10.08	LSER	10.4	*b* (CN-MeOH)	10.4
*PC*1/R_M (C18-MeOH)	10.08	*PC*1/R_M (C18-MeOH)	10.72	*PC*1/R_M (C18-MeOH)	10.72
b (CN-MeOH)	10.24	*b* (CN-MeOH)	10.72	miLogP	10.88
mR_M (C18-MeOH)	10.4	mR_M (C18-MeOH)	10.88	KOWIN	11.04
AClogP	10.56	AClogP	11.04	mR_M (C18-MeOH)	11.04
KOWIN	10.72	C_0 (C18-MeOH)	11.04	AClogP	11.36
C_0 (C18-MeOH)	11.2	KOWIN	11.2	C_0 (C18-MeOH)	11.36
ACDlogP	11.68	ALOGPs	12.32	ACDlogP	12.16
MLOGP	11.68	MLOGP	12.32	ALOGPs	12.48
ALOGPs	12.32	ACDlogP	12.48	ALOGP	12.96
ALOGP	12.96	mR_M (C18-MeCN)	12.96	MLOGP	13.12
XLOGP2	13.28	ALOGP	13.12	XLOGP2	13.28
mR_M (C18-MeCN)	13.44	*PC*1/R_M (C18-MeCN)	13.28	mR_M (C18-MeCN)	13.6
*PC*1/R_M (C18-MeCN)	13.76	XLOGP2	13.44	*PC*1/R_M (C18-MeCN)	13.92
R_M^0 (C18-MeCN)	14.08	C_0 (C18-MeCN)	14.24	R_M^0 (C18-MeCN)	14.4
C_0 (C18-MeCN)	14.88	R_M^0 (C18-MeCN)	14.4	C_0 (C18-MeCN)	14.88
C_0 (CN-MeOH)	17.76	C_0 (CN-MeCN)	16.96	C_0 (CN-MeOH)	17.44
C_0 (CN-MeCN)	17.76	C_0 (CN-MeOH)	17.44	mR_M (CN-MeOH)	17.6
mR_M (CN-MeOH)	18.08	mR_M (CN-MeOH)	17.6	C_0 (CN-MeCN)	17.6
*PC*1/R_M (CN-MeOH)	18.56	*PC*1/R_M (CN-MeOH)	18.08	mR_M (CN-MeCN)	17.92
mR_M (CN-MeCN)	18.72	mR_M (CN-MeCN)	18.08	*PC*1/R_M (CN-MeOH)	18.4
R_M^0 (C18-MeOH)	19.04	PC1/RM (CN-MeCN)	18.72	*PC*1/R_M (CN-MeCN)	18.72
*PC*1/R_M (CN-MeCN)	19.36	R_M^0 (C18-MeOH)	19.36	R_M^0 (C18-MeOH)	19.36
R_M^0 (CN-MeCN)	20.96	R_M^0 (CN-MeCN)	20.16	R_M^0 (CN-MeCN)	20.64
b (CN-MeCN)	25.76	*b* (CN-MeCN)	25.92	*b* (CN-MeCN)	26.4
AB/LogP	28.48	AB/LogP	28.64	AB/LogP	28.64
b (C18-MeOH)	35.68	*b* (C18-MeOH)	36.16	*b* (C18-MeOH)	35.84
b (C18-MeCN)	46.24	*b* (C18-MeCN)	46.72	*b* (C18-MeCN)	46.72

Table S4b Generalized pairwise correlation method – with conditional exact probability weighted ranking (GPCM-CEPW); Scores of chromatographic and *in silico* lipophilicity measures using different data pretreatment methods: standardization (St), range scaling (Rg) and ranking (Rk)

St		**Rg**		**Rk**	
logK_{OW} (exp)	9.28	logK_{OW} (exp)	9.12	logK_{OW} (exp)	9.12
miLogP	9.30	R_M^0 (CN-MeOH)	9.82	R_M^0 (CN-MeOH)	11.13
R_M^0 (CN-MeOH)	9.31	*PC*1/R_M (C18-MeOH)	10.51	b (CN-MeOH)	11.16
*PC*1/R_M (C18-MeOH)	9.97	miLogP	11.19	ClogP	11.17
b (CN-MeOH)	10.01	mR_M (C18-MeOH)	11.22	*PC*1/R_M (C18-MeOH)	11.83
ClogP	10.02	*b* (CN-MeOH)	11.92	mR_M (C18-MeOH)	11.86
mR_M (C18-MeOH)	10.67	ClogP	12.57	miLogP	13.22
LSER	12.11	XLOGP3	13.28	LSER	13.89
XLOGP3	14.12	LSER	14.64	AClogP	14.59
AClogP	14.12	AClogP	15.33	C_0 (C18-MeOH)	15.26
KOWIN	14.13	C_0 (C18-MeOH)	15.34	XLOGP3	15.92
C_0 (C18-MeOH)	14.14	KOWIN	16.02	KOWIN	16.60
ALOGPs	18.22	ALOGPs	16.72	ALOGPs	16.61
mR_M (C18-MeCN)	19.64	mR_M (C18-MeCN)	17.37	mR_M (C18-MeCN)	19.97
MLOGP	19.54	*PC*1/R_M (C18-MeCN)	19.43	ACDlogP	19.96
ACDlogP	20.26	MLOGP	20.11	R_M^0 (C18-MeCN)	20.64
*PC*1/R_M (C18-MeCN)	20.35	ALOGP	20.87	*PC*1/R_M (C18-MeCN)	21.33
R_M^0 (C18-MeCN)	21.01	R_M^0 (C18-MeCN)	21.53	ALOGP	21.34
ALOGP	21.01	ACDlogP	22.23	MLOGP	22.68
XLOGP2	23.86	C_0 (C18-MeCN)	22.25	XLOGP2	24.73
C_0 (C18-MeCN)	24.52	XLOGP2	25.08	C_0 (C18-MeCN)	25.41
mR_M (CN-MeOH)	34.35	mR_M (CN-MeOH)	34.84	mR_M (CN-MeOH)	35.06
C_0 (CN-MeCN)	35.06	C_0 (CN-MeCN)	35.54	C_0 (CN-MeCN)	35.76
mR_M (CN-MeCN)	35.06	mR_M (CN-MeCN)	35.55	mR_M (CN-MeCN)	35.76
C_0 (CN-MeOH)	35.05	C_0 (CN-MeOH)	35.53	C_0 (CN-MeOH)	35.75
*PC*1/R_M (CN-MeCN)	35.06	*PC*1/R_M (CN-MeCN)	35.55	*PC*1/R_M (CN-MeCN)	35.76
R_M^0 (C18-MeOH)	35.06	R_M^0 (C18-MeOH)	35.57	R_M^0 (C18-MeOH)	35.77
*PC*1/R_M (CN-MeOH)	35.76	*PC*1/R_M (CN-MeOH)	36.26	*PC*1/R_M (CN-MeOH)	36.45
R_M^0 (CN-MeCN)	40.65	R_M^0 (CN-MeCN)	41.11	R_M^0 (CN-MeCN)	41.25
AB/LogP	42.73	*b* (CN-MeCN)	43.23	AB/LogP	43.28
b (CN-MeCN)	42.75	AB/LogP	43.23	*b* (CN-MeCN)	43.30
b (C18-MeOH)	44.84	*b* (C18-MeOH)	45.32	*b* (C18-MeOH)	45.35
b (C18-MeCN)	46.24	*b* (C18-MeCN)	46.72	*b* (C18-MeCN)	46.72

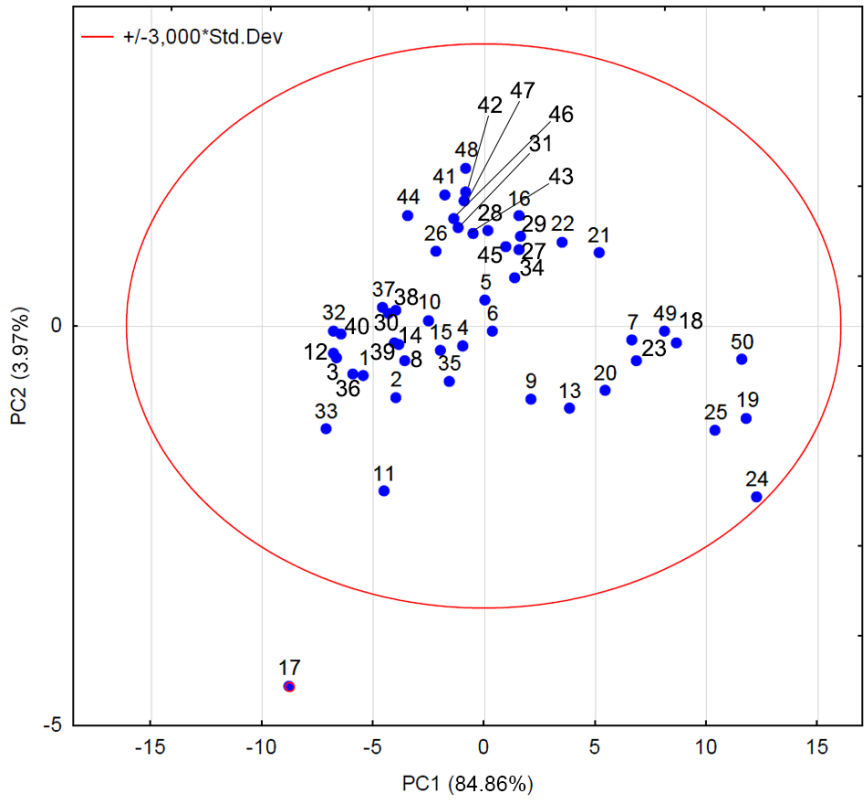

Figure S1 Principal component score plot showing disposition of the studied compounds. Two principal components are describing 88.79% of the overall data variability

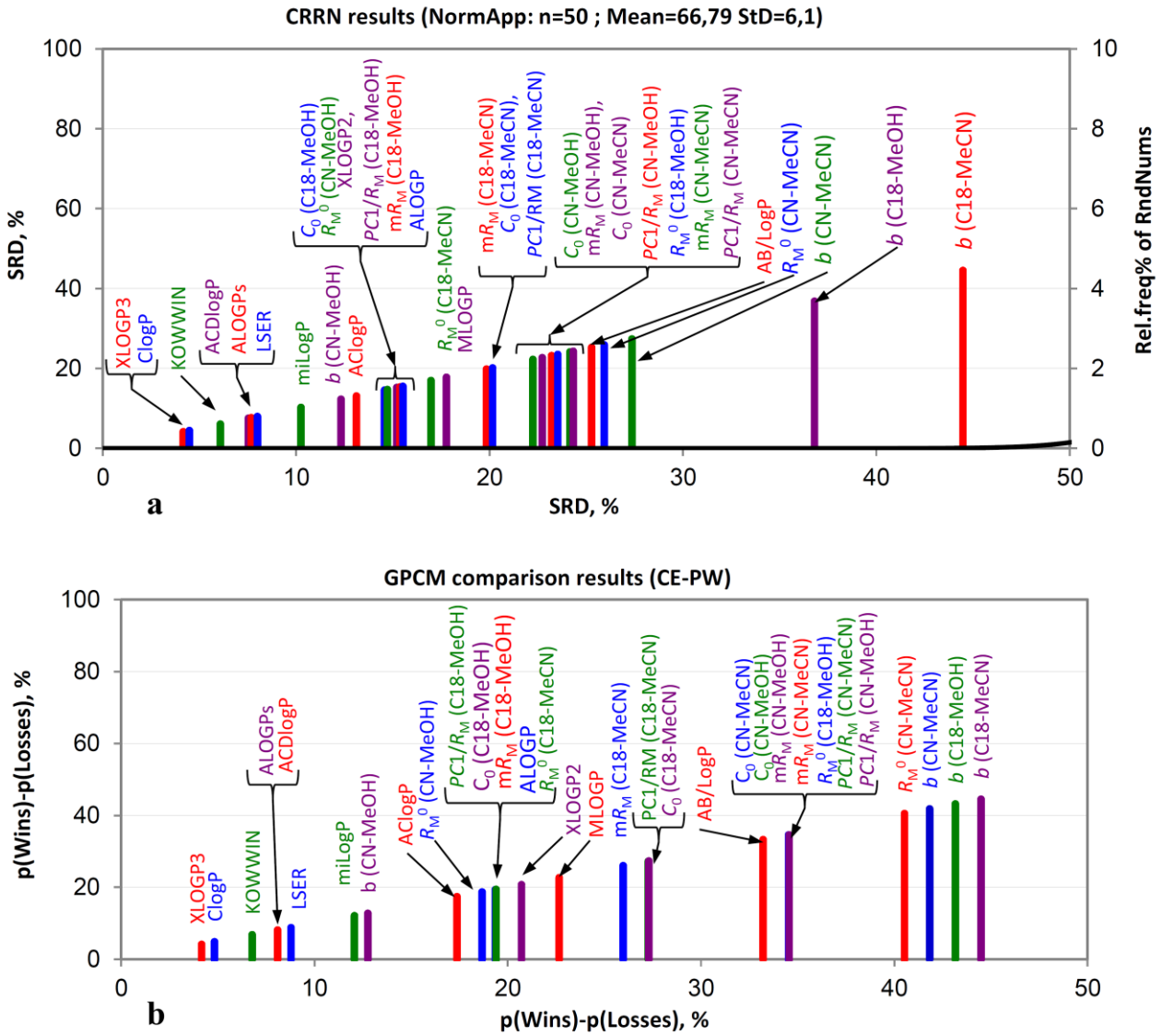

Figure S2 Comparison, ranking and grouping of chromatographic and *in silico* lipophilicity measures by SRD-CRRN (a), and GPCM-CEPW ranking (b) using was logK_{OW}(exp) as benchmark; CEPW stands for probability weighted ranking (PW) based on Fisher's conditional exact test (CE).

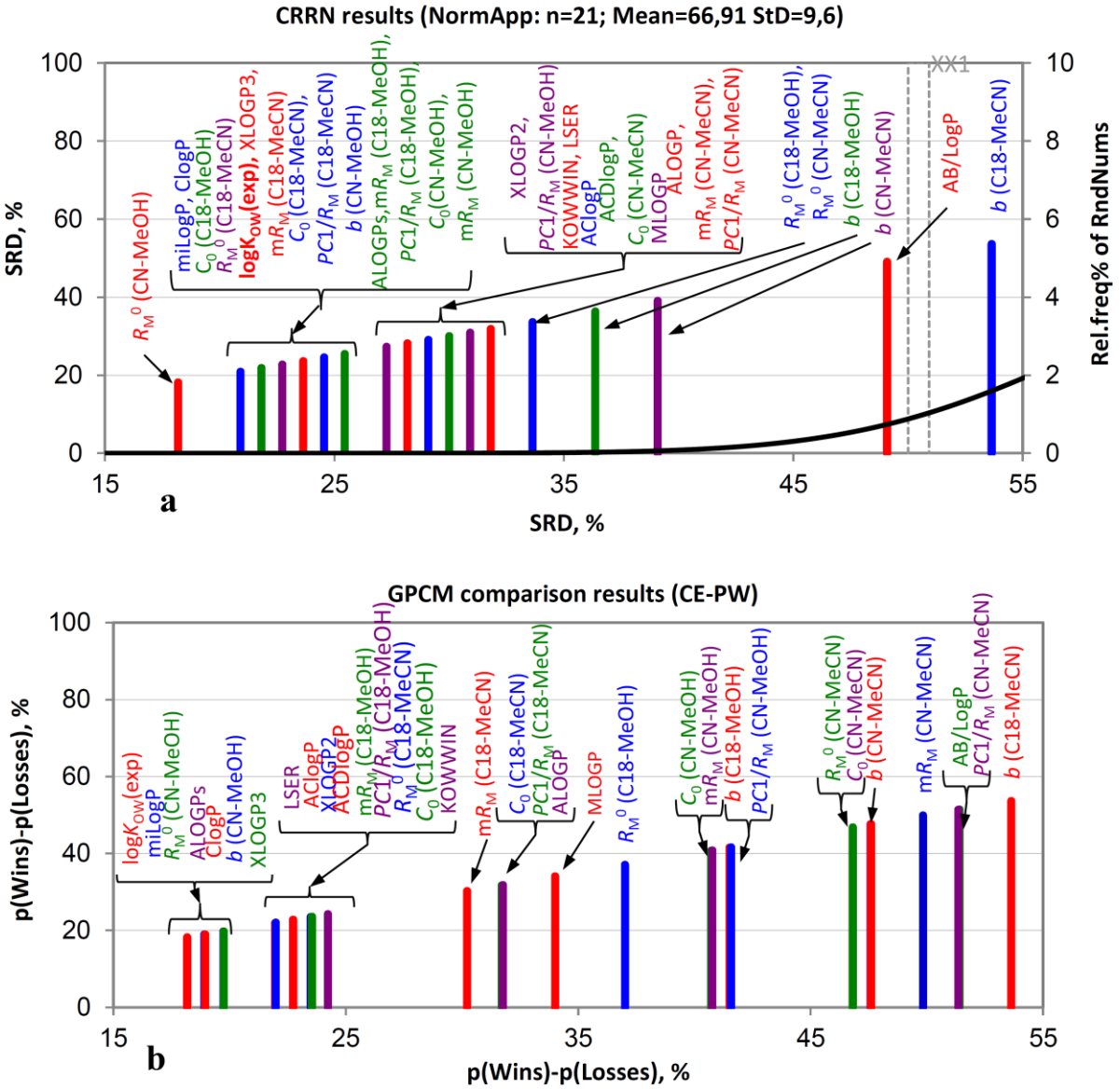

Figure S3 Comparison, ranking and grouping of chromatographic and *in silico* lipophilicity measures by SRD-CRRN (a), and GPCM-CEPW ranking (b) using set of compounds with logK_{OW} < 3 determined by the shake-flask procedure; the benchmark was the arithmetic mean average; CEPW stands for probability weighted ranking (PW) based on Fisher's conditional exact test (CE).

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